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EDITORIAL

Effect-oriented environmental analysis

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How can we deal with the roughly 100,000 chemicals in daily use, of which a significant number potentially enter the environment through point sources like wastewater treatment plants, landfills and superfund sites, and due to diffuse input through, e.g., surface run-off from agricultural and urban surfaces, or atmospheric deposition? And how can we assess the risks posed by the presence of these chemicals in an ecosystem and define quality criteria?

The classical approach is to measure environmental concentrations of as many chemicals of interest as possible with limits of detection that are as low as technically achievable. The selection of chemicals monitored was determined by the physicochemical properties of the target analytes, which up to the 1990s had to be volatile and thermally stable for GC analysis. With the introduction of electrospray ionization less than twenty years ago, all of a sudden thermolabile, polar and ionic compounds of up to 100,000 Da could be analyzed by mass spectrometry. This opened up a whole new field of environmental research, because (among others) pharmaceuticals, personal care products and the latest generation of pesticides became amenable for MS analysis.

However, the universe of chemicals keeps expanding because of the need to include metabolites and transformation products when evaluating the risk from a certain chemical. This is why researchers have started to focus on the effects of chemicals or environmental samples rather than the concentrations of chemicals in the environment, by introducing the concept of tiered testing. This effect-oriented approach allows us to focus on environmental samples that can cause negative effects in, for instance, aquatic organisms. Many biological endpoints have been proposed that range from the overall conditions of single cells or higher organisms, reflected in their growth, photosynthetic yield, proliferation or mortality, to very specific effects, such as disruption of the endocrine system (see Lutz et al., this issue) or mutagenicity. When testing full extracts of a given sample, matrix effects can prevent a clear readout, which is why a sample is very often separated into fractions of increasing lipophilicity. This reduces matrix effects and on the other hand allows us to identify i) the presence of antagonists present in the full extract, ii) the synergism, and iii) the concentration additivity of compounds with the same mode of action. Effect-oriented analysis not only helps us to focus on samples that have an effect on a chosen endpoint, but more importantly allows testing to be performed without prior knowledge of which chemicals to expect, as outlined by Brack et al. (this issue). The identification of unknown toxicants selected based on their effects has only become possible because modern mass spectrometers enable very sensitive determinations of accurate masses over very short cycle times, a prerequisite for assigning elemental compositions to precursors and fragment ions of unknown compounds found in active samples or fractions thereof.

Seiler et al. (this issue) discuss issues related to sample handling and extraction. While the choice of the biological endpoint is crucial, the way that the chemicals are extracted is also important, because they can degrade or undergo chemical reactions. Furthermore, their bioavailability depends on their speciation, which is influenced by other compounds extracted along with the toxicant. Even so, bioassays have become a very popular way to test for chemicals, as demonstrated by Reinen et al. (this issue),

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who analyzed the estrogenic potential of chemicals in an estrogen receptor affinity assay. Using a different assay, Farre et al. (this issue) showed that effect analysis is a versatile tool for monitoring transformation processes in a technical system. This was further underlined by the work done by Wenger et al. (this issue), who followed the elimination of estrogenicity in diesel exhaust by various catalytic particulate filters.

Finally, Keiter et al. investigated possible causes of the decline in fish populations in the Danube River. Even though the water quality of the river has improved over the years, PAHs are still found in high concentrations in the sediment. Using an aryl hydrocarbon receptor-based assay, they found AhR activity that could not be explained by priority pollutants. This is a case where wrong conclusions would have been drawn if only chemical analysis had been performed on the samples, and it is also an excellent example of the power of effect-oriented analysis.

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